

Momentum Representation of Coulomb Wave Functions and Level Shifts in Bottomonium due to Charm Effects

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Abstract

Since effective potentials derived from Feynman diagrams are naturally given in momentum space, we formulate the non-relativistic Coulomb problem entirely in momentum representation. We give momentum wave functions for all quantum numbers in one-dimensional integrals, even though they can be evaluated. Angular momentum decomposed Green's functions are then compactly represented. We apply this formalism to investigate the next to next leading order charm effects on 1S bottomonium level shift. Our one insertion results are given completely in analytic form and numerically agree with previous results. Our two insertion results are also in agreement. The net effect of finite charm mass is to decrease the bottom mass by 33 MeV, as determined through the measured 1S energy.

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I. INTRODUCTION

It is a common belief that new physics most likely will be due to new dynamics at a higher scale. Upon accepting this premise, we should expect that bigger effects will appear in processes in which known heavy particles, such as the bottom quark, the top quark and the Higgs boson actively participate. Such interplay between scales can be quite intricate, as exemplified in the ρ -parameter and in quite a few rare B decays. We would like on the one hand to use some of these processes to determine the masses of the known heavy particles as best as we can because the rates of many interesting processes depend on them strongly and on the other to lay the ground work to look for discrepancies as a byway to new physics. It is incumbent on us that for such processes the known dynamics must be well understood and that the so far uncalculable effects be well accounted for or at least be under control.

One active area is the first few of bottomonium energy levels [1] and the production threshold of $t\bar{t}$ [2]. Here as the starting approximation, the heavy quarks move under a color Coulomb potential non-relativistically. Because retardation is small, one can add other effective interaction pieces as perturbations by integrating out the fast degrees of freedom. One can then extract out the bottom mass from the first couple of measured energy levels. For the top quark, it decays too fast to have real bound states, but these would-be bound states have strong effects on the shape of the production cross section near the thresholds.

In the zeroth order approximation, such systems are just like a hydrogen atom. In most of the treatments of quarkonium systems, Coulomb-like wave functions in the coordinate space are used to evaluate matrix elements. We would like to ask whether an alternative may be also viable, for the reason that when one treats such systems in conjunction with quantum field theory, most if not all radiative correction calculations are done in momentum space via Feynman diagrams at some stage. In an effective Lagrangian approach, the Wilson coefficients are calculated in momentum space, but the operators are customarily converted back into coordinate space and their matrix elements are then obtained by averaging with spatial wave functions. It is therefore of some interest to see how to bypass the last step by following the momentum approach throughout.

Needless to say, hydrogen wave functions in momentum representation have been repeatedly used [3] for a long time. One difference we want to make here is that we have

a convenient and compact representation for them in one-dimensional integrals, which we shall keep in such a form even though they can be evaluated into Gegenbauer polynomials. Matrix elements can then be evaluated mostly by the use of the method of residues and the result will collapse into only a small number of terms. We shall also give a very simple representation for the propagators.

As we indicated earlier, we find it intriguing to explore the interplay of masses. Therefore, we shall use as an example to apply the momentum technique to investigate the charm mass effects [4 – 8] on the bottomonium level shifts to the next-next leading order. One notices that the binding momentum $\approx \frac{4}{3}\alpha_s m_b \approx 2 \text{ GeV}$ is comparable to $m_c \approx 1.25 \text{ GeV}$. One must take the charm loop as a whole as a term in the potential, which becomes highly non-trivial in the coordinate space.

There are two sets of diagrams. The first set is due to the insertions of the lowest order charm loop once or twice, or the limiting zero mass particle effects and a charm loop each once on the same gluon line (Fig.(1)). Also, there are diagrams due to the fourth order charm loop. (We neglect the charm loop effects on the vertex.) We have been able to evaluate all of them analytically into simple functions. They account for 98% of the charm effects for the 1S level shift. The second set is due to double insertions of the above potential on two separate gluon lines (Fig.(2)) and so far can be given only in terms of some simple integrals. The results are in agreement with those given in [6]. Furthermore, because we have the explicit functions for the first set at hand, we can follow the relevant branch of the functions and continue them to cover the toponium would-be bound state energy level shifts, here due to the bottom quark mass effects. We hope that this example is convincing enough to illustrate that the same technique can be used to cover exotic particle effects, when called upon.

In an article [9] co-authored by one of us, we showed how the technique presented here could be extended to yield results at least for the spherically symmetrical states of the hydrogen atom and gave a bound on the non-commutative scale in a certain extension of the non-relativistic kinematics [10], by using the highly accurate 1S-2S energy difference.

The plan of this paper is as follows: in the next section, we shall solve for the momentum wave functions. An operator algebra [11] will be used to normalize them. These wave

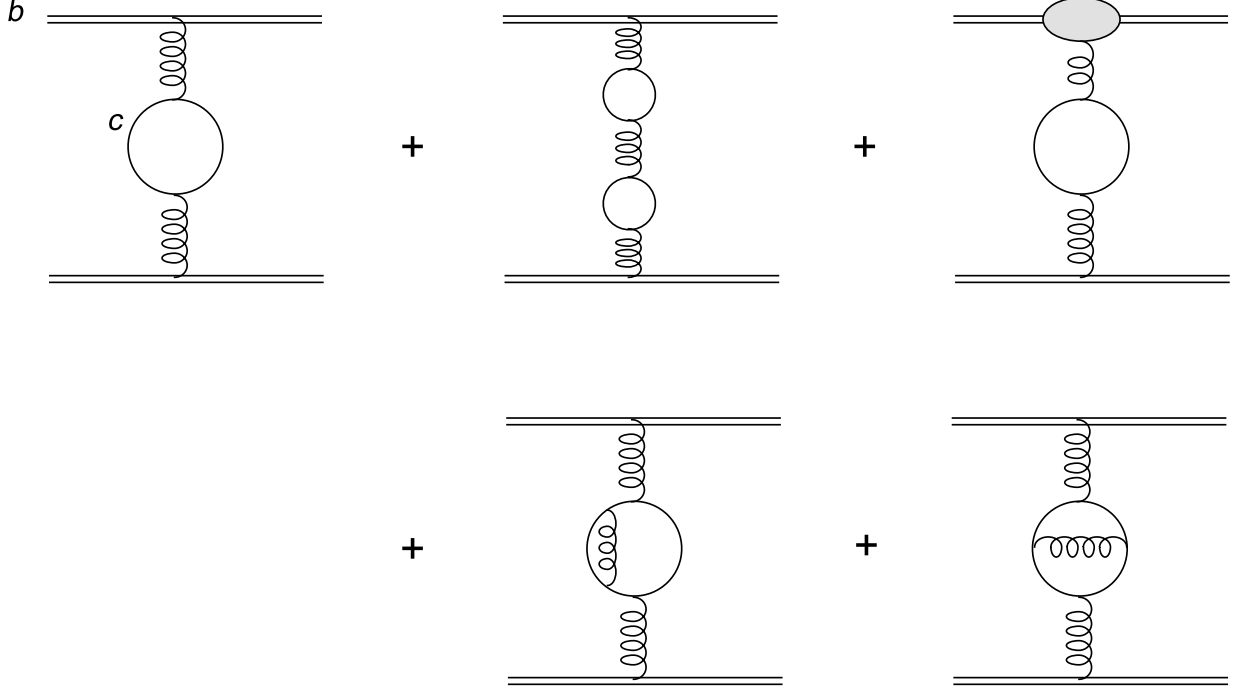


FIG. 1: We show schematically the next leading order and next-to-next leading order charm mass effects in single insertions which alter the bottomonium energy levels. The loops are composed of a charm and anti-charm pair, the shaded ellipses represent cumulative second order zero mass quark and gluon effects, and the double lines depict either a b or \bar{b} quark.

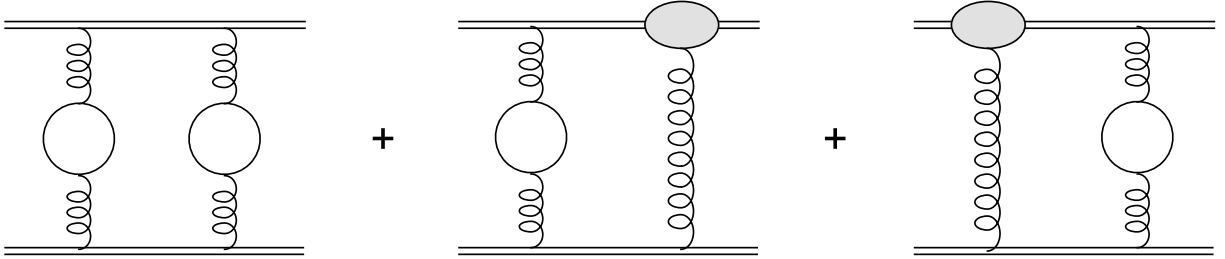


FIG. 2: We show schematically the next-to-next leading order charm effects in double insertions which alter the bottomonium energy levels. The loops are composed of a charm and anti-charm pair, the shaded ellipses represent cumulative second order zero mass quark and gluon effects, and the double lines depict either a b or \bar{b} quark.

functions in one dimensional integral representation will be the basis for our calculations later. In section 3, we shall briefly display the Green's functions for arbitrary angular momentum, but the complete treatment is devoted to the S state, as we shall use it in a subsequent section. Our momentum wave functions will be used in section 4A to obtain the ground state energy level shifts for 1S bottomonium due to next leading and next to

next leading order charm mass effects in single insertions. We are able to give our results completely analytically in simple functions. They agree with what were obtained partially analytically by others. In section 4B, we give our formulation for double insertions and carefully state our subtraction procedure. A simple test is to apply it to obtain the ground state energy level of the modified Coulomb potential $-\frac{4}{3}\alpha_s(1+\delta)\frac{1}{r}$, the exact result of which is known a priori. Numerical analysis is presented in section 5 and some concluding remarks are made in section 6. In an appendix, we further illustrate our formalism by evaluating some well known matrix elements of $(\frac{1}{r})^{0,1,2}$.

II. MOMENTUM WAVE FUNCTIONS

In this section, we shall derive a one-dimensional representation for the color Coulomb wave functions and show that, when converted back into coordinate space, they are the same as in textbooks. In fact, they will be slightly more general, because in some cases where the perturbing potential has power law dependence on the radial coordinate, we can take care of it easily. We shall use an algebra to determine the normalization factors

From the Schrodinger equation, with the reduced mass $m = m_b/2$ for bottomonium,

$$[E - \frac{1}{2m}(\frac{1}{i}\frac{\vec{\partial}}{\partial\vec{\xi}})^2 + \frac{4}{3}\alpha_s\frac{1}{\sqrt{\xi^2}}]\psi(\vec{\xi}) = 0, \quad (1)$$

we take away the centrifugal barrier and perform an angular momentum decomposition

$$\psi(\vec{\xi}) = Y_{l,m}(\theta,\phi)\tilde{\gamma}_l(\xi)\xi^{-(l+1)}, \quad (2)$$

to obtain

$$[(E - \frac{1}{2m}(\frac{1}{i}\frac{d}{d\xi})^2)\xi - \frac{i}{m}(l+1)(\frac{1}{i}\frac{d}{d\xi}) + \frac{4}{3}\alpha_s]\tilde{\gamma}_l(\xi) = 0. \quad (3)$$

We have used $\vec{\xi}$ to denote coordinates, with ξ as the radial distance and θ, ϕ as the angles. Now we perform a Fourier transform with respect to the *radial distance* ξ

$$\tilde{\gamma}_l(\xi) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} dp e^{ip\xi} \gamma_l(p) \quad (4)$$

to arrive at [12]

$$[(E - \frac{p^2}{2m})i\frac{d}{dp} - \frac{i}{m}(l+1)p + \frac{4}{3}\alpha_s]\gamma_l(p) = 0. \quad (5)$$

Let us denote the energy of the state as

$$E = \frac{p_0^2}{2m}, \quad (6)$$

and rearrange the equation into

$$\left(\frac{d}{dp} + \frac{l+1+i\eta}{p-p_0} + \frac{l+1-i\eta}{p+p_0}\right)\gamma_l = 0, \quad (7)$$

where we have written

$$\eta = \frac{4}{3}\alpha_s \frac{m}{p_0}. \quad (8)$$

The solution of this equation is

$$\gamma_l(p) = A_l \frac{1}{(p-p_0)^{l+1+i\eta}} \frac{1}{(p+p_0)^{l+1-i\eta}}, \quad (9)$$

where A_l is an integration constant to be determined shortly by normalization. The bound states are determined by the poles in the upper p-plane. Thus for the negative energy solutions we set

$$p_0 = i\kappa, \quad \eta = -in, \quad (10)$$

in which we require

$$n - l - 1 = r = 0, 1, 2, \dots \quad (11)$$

so that there is no pole in the lower p-plane. We do not want to burden our expressions in the remainder of this section with indices and therefore it is understood that we shall deal with states with the same principal quantum number n one at a time.

To determine A_l , we go back to the coordinate representation, where we notice that

$$u_l(\xi) \equiv \xi^{-l} \tilde{\gamma}_l(\xi) \quad (12)$$

satisfies the equation

$$H_l u_l = E u_l, \quad (13)$$

where

$$H_l \equiv \frac{p^2}{2m} + \frac{l(l+1)}{2m\xi^2} - \frac{4}{3}\alpha_s \frac{1}{\xi}, \quad p \equiv \frac{1}{i} \frac{d}{d\xi}. \quad (14)$$

Let us consider the operator [11]

$$L_l \equiv p - i\left(\frac{l}{\xi} - \frac{4}{3}\alpha_s \frac{m}{l}\right). \quad (15)$$

Some straightforward algebra shows that we have

$$L_l H_l - H_{l-1} L_l = 0. \quad (16)$$

It follows that if u_l is an eigenvector of H_l , so is $L_l u_l$ of H_{l-1} , i.e. if the eigenenergy is E_0 ,

$$H_l u_l = E_0 u_l, \quad (17)$$

then

$$L_l H_l u_l = H_{l-1} L_l u_l \rightarrow E_0 (L_l u_l) = H_{l-1} (L_l u_l). \quad (18)$$

E_0 as well known depends only on n but not l for bound states. One can easily arrive at

$$\frac{1}{2m} L_l^\dagger L_l = H_l + \left(\frac{4}{3}\alpha_s\right)^2 \frac{m}{2l^2}. \quad (19)$$

Therefore, for a given n , L_l acts as a lowering operator

$$L_l u_l = B_l u_{l-1}, \quad (20)$$

which gives a norm

$$\frac{1}{2m} |B_l|^2 = \left(\frac{4}{3}\alpha_s\right)^2 \frac{m}{2} \left(\frac{1}{l^2} - \frac{1}{n^2}\right), \quad (21)$$

upon using the bound state energies

$$E_0 = -\left(\frac{4}{3}\alpha_s\right)^2 \frac{m}{2n^2}. \quad (22)$$

We shall follow the conventional choice to make the wave functions u_l real, which dictates the choice of the phase for B_l so that

$$L_l u_l = -i \frac{1}{a} \sqrt{\frac{1}{l^2} - \frac{1}{n^2}} u_{l-1}, \quad a^{-1} \equiv \frac{4}{3} \alpha_s m. \quad (23)$$

When we transcribe this last equation into the momentum representation, we have

$$\frac{1}{a} \sqrt{\frac{1}{l^2} - \frac{1}{n^2}} i \frac{d}{dp} \gamma_{l-1} = \left(ip - \frac{1}{la}\right) \gamma_l. \quad (24)$$

Upon using the explicit solutions for $\gamma(p)$'s, we arrive at

$$A_l = -\frac{2}{na} \sqrt{n^2 - l^2} A_{l-1}, \quad (25)$$

and upon iteration

$$A_l = (-2\kappa)^l \sqrt{\frac{(n+l)!}{n(n-l-1)!}} A_0. \quad (26)$$

We have used the relation

$$\kappa = \frac{1}{na}, \quad (27)$$

and in conformity with the standard choice of phase, we fix

$$A_0 = -\sqrt{\frac{2\kappa^3}{\pi}}. \quad (28)$$

At this point we want to be reminded that the radial wave functions are $\tilde{\gamma}_l(\xi)\xi^{-(l+1)}$. Because we shall use them to evaluate matrix elements of operators which may have ξ dependence, let us define more generally

$$\frac{\tilde{\gamma}_l(\xi)}{\xi^t} \equiv \tilde{\gamma}_l^t(\xi), \quad (29)$$

the Fourier transform of which

$$\tilde{\gamma}_l^t(\xi) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} dp e^{ip\xi} \gamma_l^t(p) \quad (30)$$

satisfies

$$i \frac{d}{dp} \gamma_l^t(p) = \gamma_l^{t-1}(p), \quad (31)$$

and therefore

$$(i \frac{d}{dp})^t \gamma_l^t(p) = \gamma_l^0(p) \equiv \gamma_l(p). \quad (32)$$

It can be inverted to yield

$$(i)^t \gamma_l^t(p) = (-1)^{t+1} \frac{1}{(t-1)!} \int_{-\infty}^0 dp' p'^{t-1} A_l \frac{(p' + p + p_0)^{n-l-1}}{(p' + p - p_0)^{n+l+1}}, \quad (33)$$

for a given n and $t \geq 1$. This is the basic integral representation we shall use, although it can be evaluated into Gegenbauer polynomials.

To proceed further, we want to write Laguerre polynomials L_r^k in an integral representation over momentum. From the definition of $\tilde{\gamma}(\xi)$ and how L_r^k appears in the wave function, i.e.

$$\begin{aligned}\psi_{nlm} &= Y_{lm}(\theta, \phi) \frac{\tilde{\gamma}_l}{\xi^{l+1}} \\ &= Y_{lm}(\theta, \phi) \sqrt{(2\kappa)^3 \frac{(n-l-1)!}{2n(n+l)!}} e^{-\kappa\xi} (2\kappa\xi)^l L_r^k(2\kappa\xi),\end{aligned}\quad (34)$$

where $r = n - l - 1$ and $k = 2l + 1$, we have

$$\begin{aligned}L_r^k(\rho \equiv 2\kappa\xi) &= -\frac{(r+k)!}{r!} \frac{1}{(k-1)!} e^{\kappa\xi} \int_{-\infty}^0 dp' p'^{k-1} \\ &\quad \times \frac{1}{2\pi i} \int_{-\infty}^{\infty} dp e^{ip\xi} \frac{(p+p'+p_0)^r}{(p+p'-p_0)^{r+k+1}}.\end{aligned}\quad (35)$$

One can of course carry out the p and p' integrations to obtain

$$L_r^k(\rho) = \frac{e^\rho}{r!} \rho^{-k} \left(\frac{d}{d\rho}\right)^r \rho^{r+k} e^{-\rho}.\quad (36)$$

However, for some problem where a sum over r has to be performed, it is more useful to have L_r^k presented as in Eq. (35).

Before we leave this section, we give a formula which is useful in the calculation of matrix elements,

$$\int_0^\infty dp_1 dp_2 \frac{p_1^i p_2^j}{(p_1 + p_2 + b)^k} = \frac{\Gamma(i+1)\Gamma(j+1)}{\Gamma(i+j+2)} \int_0^\infty dp' \frac{p'^{i+j+1}}{(p' + b)^k},\quad (37)$$

when $k > i + j + 2$. In an appendix, we shall use it to reproduce some of the classic matrix elements to illustrate further our formalism.

III. PROPAGATORS

In order to carry out double insertions for the next-next leading order energy shifts, we need the propagators which are defined in

$$G(\vec{x}, \vec{y}; E) \equiv -\sum_i \frac{|i \rangle \langle i|}{E - E_i} = \sum_l (2l+1) G_l(x, y; E) P_l\left(\frac{\vec{x} \cdot \vec{y}}{xy}\right),\quad (38)$$

where P_l are the Legendre polynomials and please note the minus sign in the sum over the eigen-energies E_i . We have assumed a central (Coulomb) potential in writing down the above expression. Because of an interesting result in angular momentum decomposed Green's functions [13], we make a slight change of notation and write the energy as

$$E = -\kappa_0^2/m_b = p_0^2/m_b, \quad (39)$$

then

$$\begin{aligned} G_l(x, y; E) &= \frac{m_b \kappa_0}{2\pi} (2\kappa_0 x)^l (2\kappa_0 y)^l e^{-\kappa_0(x+y)} \sum_{r=0}^{\infty} \frac{L_r^{2l+1}(2\kappa_0 x) L_r^{2l+1}(2\kappa_0 y) r!}{(r+l+1-\nu)(r+2l+1)!} \\ &= \frac{m_b \kappa_0}{2\pi} \sum_{n=1}^{\infty} \frac{2n}{(2\kappa_0)^3} \frac{1}{n-\nu} \frac{u_n^l(2\kappa_0 x)}{x} \frac{u_n^l(2\kappa_0 y)}{y}, \end{aligned} \quad (40)$$

where we have restored the principal quantum number n to label the radial wave functions (i.e. $u_l \rightarrow u_n^l$) and defined

$$\nu \equiv \frac{m_b}{2\kappa_0} \left(\frac{4}{3} \alpha_s \right). \quad (41)$$

We shall later on be interested in the behavior $\nu \rightarrow 1$ when we look into the ground state. Now because of Eq.(35), which gives the reduced radial functions

$$\begin{aligned} \frac{u_n^l(2\kappa_0 x)}{x} &= (i)^{-(l+1)} (-1)^l \frac{1}{l!} A_l \left(\frac{1}{2\pi} \right)^{1/2} \\ &\times \int_{-\infty}^{\infty} dp_1 e^{ip_1 x} \int_{-\infty}^0 dp'_1 p_1^l \frac{(p'_1 + p_1 + p_0)^{n-l-1}}{(p'_1 + p_1 - p_0)^{n+l+1}}, \end{aligned} \quad (42)$$

and a similar expression for $\frac{u_n^l(2\kappa_0 y)}{y}$, with $p_1 \rightarrow p_2$ and $p'_1 \rightarrow p'_2$. Also, we write

$$\frac{1}{n-\nu} = \int_0^1 d\rho \rho^{n-\nu-1}, \quad (43)$$

assuming $1-\nu > 0$. Performing the sum over n in Eq.(40), we find

$$\begin{aligned} G_l(x, y; E) &= (-1)^l \frac{m_b (2\kappa_0)^k}{4\pi} \frac{k!}{(l!)^2} \left(\frac{1}{2\pi i} \right)^2 \int_{-\infty}^{\infty} dp_1 e^{ip_1 x} \int_{-\infty}^{\infty} dp_2 e^{ip_2 y} \\ &\times \int_{-\infty}^0 dp'_1 p_1^l \int_{-\infty}^0 dp'_2 p_2^l \int_0^1 d\rho \rho^{l-\nu} \\ &\times \frac{1}{((p_1 + p'_1 - p_0)(p_2 + p'_2 - p_0) - \rho(p_1 + p'_1 + p_0)(p_2 + p'_2 + p_0))^{k+1}}, \\ &k \equiv 2l+1. \end{aligned} \quad (44)$$

For the case $l = 0$, it is easy to perform the sum and integrate over p'_1, p'_2 to obtain

$$G_{l=0}(x, y; E) = \frac{-m_b}{8\pi\kappa_0} \left(\frac{1}{2\pi i}\right)^2 \int_{-\infty}^{\infty} dp_1 e^{ip_1 x} \int_{-\infty}^{\infty} dp_2 e^{ip_2 y} \times \int_0^1 d\rho \rho^{-1-\nu} \ln\left(\frac{bc}{ad}\right), \quad (45)$$

where

$$bc = (p_1 - p_0)(p_2 - p_0) - \rho(2p_1 p_2 - 2p_0^2) + \rho^2(p_1 + p_0)(p_2 + p_0), \quad (46)$$

and

$$ad = bc - 4\rho p_0^2. \quad (47)$$

With the wave functions and the propagators, we can proceed to calculate energy shifts in the next sections.

IV. ENERGY SHIFTS DUE TO CHARM EFFECTS

One objective in high precision tests of fundamental physics is to give operational meaning to the parameters in a theory and to measure them. Among the many parameters in the Standard Model, great improvements are being made in extracting the values of heavy particle masses, both experimentally and theoretically. For example, for the b-quark mass one way to determine it is by using the ground state of the bottomonium. As for the top quark, although its life time is too short for forming toponium, the location and the shape of the $t\bar{t}$ threshold will yield crucial information.

Such considerations have been augmented to a very high and sophisticated degree by many groups. Thus, the ground state energy level of the bottomonium has been calculated to an accuracy of $\alpha_s^5(\ln(\alpha_s))$ [1]. At this order, among other contributions, there are the shifts due to the charm quark vacuum polarizations in the potential function. The important ratio here for the energy shifts is k/m_c , where k is the momentum transfer, which is $\sim \frac{2}{3}\alpha_s m_b$. Thus $k/m_c \approx 1$, in contradistinction to what is in atomic physics, where it is $\approx \alpha_{em}$. This numerical value is a cause for concern if one is to perform the intended calculation by an approximate expansion either in k/m_c or m_c/k . We must calculate effects due to these potential terms exactly. In this section, we shall show how this is handled in our formulation.

A. Potential Terms and Energy Shifts for Single Insertions

The expression for the energy shift due to a single insertion is

$$\Delta E = \int_{-\infty}^{\infty} d^3\vec{\xi} \psi(\vec{\xi})^\dagger \tilde{V}(\xi) \psi(\vec{\xi}), \quad (48)$$

with the Fourier transform

$$\tilde{V}(\xi) = \frac{1}{2\pi^2} \int_{-\infty}^{\infty} d^3k e^{i\vec{k}\cdot\vec{\xi}} V(k^2). \quad (49)$$

After introducing the momentum wave function as in Eq.(30),

$$\tilde{\gamma}_l(\xi) \xi^{-l} = (\tilde{\gamma}_l(\xi) \xi^{-l})^* = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} dp e^{ip\xi} \gamma_l^l(p), \quad (50)$$

into the spatial wave function

$$\psi(\vec{\xi}) = Y_{lm}(\Omega) \tilde{\gamma}_l(\xi) \xi^{-(l+1)}, \quad (51)$$

because the potential is spherically symmetrical, we can immediately integrate over the solid angle Ω to obtain

$$\Delta E = \frac{1}{2\pi} \int_0^\infty d\xi \int_{-\infty}^{\infty} dp_1 e^{ip_1\xi} \gamma_l^l(p_1) \tilde{V}(\xi) \int_{-\infty}^{\infty} dp_2 e^{ip_2\xi} \gamma_l^l(p_2). \quad (52)$$

At this point, we use the momentum representation of the potential in eq.(49). We write $\vec{k} \cdot \vec{\xi} = k\xi \cos\theta$ and integrate over ξ and the angles to obtain

$$\Delta E = \frac{i}{2\pi^2} \int_{-\infty}^{\infty} dp_1 \gamma_l^l(p_1) \int_{-\infty}^{\infty} dp_2 \gamma_l^l(p_2) \int_0^\infty k dk \ln\left(\frac{p_1 + p_2 + k}{p_1 + p_2 - k}\right) V(k^2) \quad (53)$$

Let us specialize and consider the energy shifts of the ground state, the wave function of which is (n=1)

$$\gamma_{l=0}^{l=0}(p) = A_0 \frac{1}{(p - i\kappa_1)^2}, \quad (54)$$

with

$$A_0 = -\sqrt{\frac{2\kappa_1^3}{\pi}}, \quad \kappa_1 = \frac{4}{3}\alpha_s m_{reduced} = \frac{2}{3}\alpha_s m_b \quad (55)$$

for a bottomonium. We can easily use the residue theorem to carry out the integrations.

We shall write as our standard form for any piece of the momentum space potential

$$V(k^2) = \frac{1}{k^2}g(k^2), \quad (56)$$

taking into account of the factor of $2\pi^2$ in Eq.(49), then it is easy to show that the corresponding energy shift is

$$\frac{1}{2\pi^2} < \frac{1}{k^2}g(k^2) > = N \int_0^\infty dk \frac{1}{(k^2 + 4\kappa_1^2)^2} g(k^2), \quad (57)$$

where the factor N is

$$N = A_0^2 16\kappa_1. \quad (58)$$

The potential pieces to account for charm effects are due to: (a) the charm loop in the lowest order

$$V_{charm}^{NLO}(k^2) = (-\frac{4}{3}\alpha_s)T_F\alpha_s\frac{2}{3\pi}(\int_1^\infty dz \frac{f(z)}{k^2 + 4m^2z^2} + \frac{1}{k^2}(-\frac{1}{2}\ln(\frac{k^2}{m^2}) + \frac{5}{6})), \quad (59)$$

where

$$f(z) = \frac{1}{z^2}\sqrt{z^2 - 1}(1 + \frac{1}{2z^2}), \quad (60)$$

(b) the iteration of the above and its combination with the zero mass quark and gluon effects [14]

$$V_{massless}^{NLO}(k^2) = (-\frac{4}{3}\alpha_s)\frac{\alpha_s}{4\pi}\frac{1}{k^2}(-\beta_0\ln(\frac{k^2}{\mu^2}) + a_1), \quad (61)$$

where

$$\beta_0 = \frac{11}{3}C_A - \frac{4}{3}T_F n_l, \quad a_1 = \frac{31}{9}C_A - \frac{20}{9}T_F n_l, \quad (62)$$

and μ is a subtraction scale, $C_A = 3$, $T_F = 1/2$ and $n_l = 4$, and (c) α_s corrections to the charm loop. In this section, the mass symbol m refers to the mass of the charm quark. We have [5, 6]

$$V_{charm}^{NNLO} = V_{charm}^{NNLO}(1) + V_{charm}^{NNLO}(2) + V_{charm}^{NNLO}(3), \quad (63)$$

where

$$\begin{aligned} V_{charm}^{NNLO}(1) = \bar{c}_1 [& \bar{a}_1 \int_1^\infty dz f(z) \frac{\ln(\frac{k^2}{4m^2})}{k^2 + 4m^2z^2} + \bar{a}_2 \int_1^\infty dz \frac{f(z)}{k^2 + 4m^2z^2} \\ & + \bar{a}_3 \frac{1}{k^2} \ln^2(\frac{k^2}{m^2}) + \bar{a}_4 \frac{1}{k^2} \ln(\frac{k^2}{m^2}) + \bar{a}_5 \frac{1}{k^2}], \end{aligned} \quad (64)$$

with

$$\begin{aligned}\bar{c}_1 &= (-4\alpha_s/3)(\frac{\alpha_s}{4\pi})(T_F\alpha_s\frac{2}{3\pi}), \\ \bar{a}_1 &= -2\beta_0, \quad \bar{a}_2 = -2\beta_0\ln(\frac{4m^2}{\mu^2}) + 2a_1, \quad \bar{a}_3 = \beta_0, \\ \bar{a}_4 &= -(5/3)\beta_0 + \beta_0\ln(\frac{m^2}{\mu^2}) - a_1, \quad \bar{a}_5 = -(5/3)\beta_0\ln(\frac{m^2}{\mu^2}) + (5/3)a_1,\end{aligned}$$

$$\begin{aligned}V_{charm}^{NNLO}(2) &= \bar{c}_2[\int_1^\infty dz_1 dz_2 \frac{k^2 f(z_1)}{k^2 + 4m^2 z_1^2} \frac{f(z_2)}{k^2 + 4m^2 z_2^2} - \int_1^\infty dz f(z) \frac{\ln(k^2/4m^2)}{k^2 + 4m^2 z^2} \\ &\quad + (-2\ln 2 + 5/3) \int_1^\infty dz \frac{f(z)}{k^2 + 4m^2 z^2} + \frac{1}{4} \frac{1}{k^2} (-\ln(k^2/m^2) + 5/3)^2], \quad (65)\end{aligned}$$

where

$$\bar{c}_2 = (-\frac{4}{3}\alpha_s)(T_F\alpha_s\frac{2}{3\pi})^2, \quad (66)$$

and

$$V_{charm}^{NNLO}(3) = \bar{c}_3 \frac{1}{k^2} [c_1 \ln(1 + \frac{k^2}{4c_2^2 m^2}) + d_1 \ln(1 + \frac{k^2}{4d_2^2 m^2}) - (\ln(\frac{k^2}{m^2}) - \frac{161}{114} - \frac{26}{19}\zeta_3)], \quad (67)$$

where

$$\bar{c}_3 = (-\frac{4}{3}\alpha_s)(\frac{\alpha_s}{4\pi})^2 (\frac{76}{3}T_F), \quad c_1 = \frac{\ln \frac{A}{d_2}}{\ln \frac{c_2}{d_2}}, \quad d_1 = \frac{\ln \frac{c_2}{A}}{\ln \frac{c_2}{d_2}}, \quad (68)$$

and

$$A = \exp(\frac{161}{228} + \frac{13}{19}\zeta_3 - \ln 2), \quad c_2 = 0.470 \pm 0.005, \quad d_2 = 1.120 \pm 0.010. \quad (69)$$

We now apply Eq.(57) to obtain energy shifts. The more tedious task in the calculation is to integrate over the spectral density $f(z)$. It turns out that all the integrals involved can be evaluated analytically into simple functions. Our method is first to assume that the parameter

$$y \equiv \frac{\kappa_1}{m} \quad (70)$$

is ≤ 1 , so that we can expand the integrand in powers of y/z . The integration over z can then be performed and the infinite series are then resummed. Since we have combinations of integrals which correspond to physical quantities and the analytic results for them, we can then unambiguously continue them into values of $y \geq 1$, which are relevant for investigating the toponium and the very light quark mass limit.

For the next to leading order, we have

$$(\Delta E)_{charm}^{NLO} = (-\frac{4}{3}\alpha_s)T_F\alpha_s\frac{2}{3\pi}\kappa_1(y^2I - (\ln(2y) - \frac{11}{6})), \quad (71)$$

where [15]

$$I = -\frac{1}{y^2}\left(\frac{2}{y^2} + \frac{11}{6}\right) - \frac{1}{(1-y^2)^{1/2}}\frac{\cos^{-1}y}{y}\left(\frac{2}{y^4} + \frac{1}{2y^2} - 1\right) + \frac{\pi}{2}\frac{1}{y^3}\left(\frac{2}{y^2} + \frac{3}{2}\right), \quad y \leq 1 \quad (72)$$

which goes to $2/5$ as $y \rightarrow 0$, reproducing the well-known QED Uehling result [16]. By analytic continuation, we have

$$I = -\frac{1}{y^2}\left(\frac{2}{y^2} + \frac{11}{6}\right) - \frac{1}{(y^2-1)^{1/2}}\frac{\ln(y+(y^2-1)^{1/2})}{y}\left(\frac{2}{y^4} + \frac{1}{2y^2} - 1\right) + \frac{\pi}{2}\frac{1}{y^3}\left(\frac{2}{y^2} + \frac{3}{2}\right), \quad y \geq 1 \quad (73)$$

which will be useful when we consider $t\bar{t}$ threshold or high Z muonic atoms. The result here agrees with what was obtained before [6].

For the next-next leading order, we just list the analytic result for each piece. They are

$$\begin{aligned} \frac{1}{2\pi^2} < \int_1^\infty dz f(z) \frac{\ln(k^2/4m^2)}{k^2 + 4m^2z^2} > &= N \int_1^\infty dz f(z) \int_0^\infty dk \frac{k^2}{(k^2 + 4\kappa_1^2)^2} \frac{\ln(k^2/4m^2)}{k^2 + 4m^2z^2} \\ &= N \frac{2}{(2m)^3} \int_1^\infty dz f(z) \int_0^\infty dk' \frac{k'^2}{(k'^2 + y^2)^2} \frac{\ln(k')}{k'^2 + z^2} \\ &= N \frac{2}{(2m)^3} \int_1^\infty dz f(z) \frac{\pi}{4y} \left[\frac{z^2 + y^2}{(z^2 - y^2)^2} \ln(y) \right. \\ &\quad \left. - \frac{2yz}{(z^2 - y^2)^2} \ln(z) + \frac{1}{z^2 - y^2} \right] \\ &= N \frac{2}{(2m)^3} \frac{\pi}{4y} \left[-2y \frac{d}{dy^2} H + (\ln(y)(2y^2 \frac{d}{dy^2} + 1) + 1) G \right], \end{aligned} \quad (74)$$

$$\frac{1}{2\pi^2} < \int_1^\infty dz f(z) \frac{1}{k^2 + 4m^2z^2} > = N \int_1^\infty dz f(z) \int_0^\infty dk \frac{k^2}{(k^2 + 4\kappa_1^2)^2} \frac{1}{k^2 + 4m^2z^2}$$

$$\begin{aligned}
&= N \frac{1}{(2m)^3} \left(\frac{\pi}{2y} \right) \int_1^\infty dz f(z) \left[\frac{y^2 - yz}{(z^2 - y^2)^2} \right] + \frac{1}{2} \frac{1}{z^2 - y^2} \\
&= N \frac{1}{(2m)^3} \left(-\frac{\pi}{4y} \right) \frac{d}{dy} (J - yG),
\end{aligned} \tag{75}$$

$$\begin{aligned}
\frac{1}{2\pi^2} < \frac{1}{k^2} \ln^2 \left(\frac{k^2}{m^2} \right) > &= N \int_0^\infty dk \frac{\ln^2 \left(\frac{k^2}{m^2} \right)}{(k^2 + 4\kappa_1^2)^2} \\
&= N \frac{\pi}{4\kappa_1^3} \left[\frac{\pi^2}{8} + \frac{1}{2} \ln^2(2y) - \ln(2y) \right],
\end{aligned} \tag{76}$$

$$\begin{aligned}
\frac{1}{2\pi^2} < \frac{1}{k^2} \ln \left(\frac{k^2}{m^2} \right) > &= N \int_0^\infty dk \frac{\ln \left(\frac{k^2}{m^2} \right)}{(k^2 + 4\kappa_1^2)^2} \\
&= N \frac{\pi}{16\kappa_1^3} [\ln(2y) - 1],
\end{aligned} \tag{77}$$

$$\begin{aligned}
\frac{1}{2\pi^2} < \frac{1}{k^2} \ln \left(1 + \frac{k^2}{4m^2 d^2} \right) > &= N \int_0^\infty dk \frac{\ln \left(1 + \frac{k^2}{4m^2 d^2} \right)}{(k^2 + 4\kappa_1^2)^2} \\
&= N \frac{\pi}{16m^3 y^2} \left[\frac{1}{y} \ln \left(1 + \frac{y}{d} \right) - \frac{1}{y + d} \right],
\end{aligned} \tag{78}$$

$$\frac{1}{2\pi^2} < \frac{1}{k^2} > = N \frac{\pi}{32\kappa_1^3}, \tag{79}$$

and

$$\begin{aligned}
&\frac{1}{2\pi^2} < \int_1^\infty dz_1 \int_1^\infty dz_2 f(z_1) f(z_2) \frac{k^2}{(k^2 + 4m^2 z_1^2)(k^2 + 4m^2 z_2^2)} > \\
&= < \int_1^\infty dz_1 \int_1^\infty dz_2 f(z_1) f(z_2) \left(\frac{1}{z_1^2 - z_2^2} \right) \left(\frac{z_1^2}{k^2 + 4m^2 z_1^2} - \frac{z_2^2}{k^2 + 4m^2 z_2^2} \right) > \\
&= N \frac{\pi}{16m^3 y} \int_1^\infty dz_1 \int_1^\infty dz_2 f(z_1) f(z_2) \left[\left(y^2 \frac{d}{dy^2} + \frac{1}{2} \right) \left(-y^2 \frac{1}{z_1^2 - y^2} \frac{1}{z_2^2 - y^2} \right) \right. \\
&\quad \left. - y \frac{d}{dy^2} \left(\frac{1}{z_1 + z_2} \frac{z_2^2}{z_2^2 - y^2} - y^2 \frac{z_1}{z_1^2 - y^2} \frac{1}{z_2^2 - y^2} \right) \right] \\
&= N \frac{\pi}{32m^3 y} \left[\left(y \frac{d}{dy} + 1 \right) (-y^2 G^2) - \frac{d}{dy} (K - y^2 GJ) \right].
\end{aligned} \tag{80}$$

The functions G, H, J, K which individually can be defined only for $y \leq 1$ are

$$\begin{aligned}
G &\equiv \int_1^\infty dz \frac{f(z)}{z^2 - y^2} \\
&= \frac{1}{y^2} \left[\left(1 + \frac{1}{2y^2}\right) \left(1 - \frac{(1-y^2)^{1/2}}{y} \sin^{-1}(y)\right) - \frac{1}{6} \right],
\end{aligned} \tag{81}$$

$$\begin{aligned}
H &\equiv \int_1^\infty dz \frac{zf(z)\ln(z)}{z^2 - y^2} \\
&= -\frac{\pi}{8y^2} [4(1-y^2)^{1/2} \ln(1 + (1-y^2)^{1/2}) - 3\ln(2) + \frac{1}{2} \\
&\quad + \frac{2}{y^2} ((1-y^2)^{1/2} \ln(1 + (1-y^2)^{1/2}) - \ln(2))],
\end{aligned} \tag{82}$$

$$\begin{aligned}
J &\equiv \int_1^\infty dz \frac{zf(z)}{z^2 - y^2} \\
&= \frac{\pi}{2} \frac{1}{y^2} \left[\frac{3}{4} - (1-y^2)^{1/2} + \frac{1}{2y^2} (1 - (1-y^2)^{1/2}) \right].
\end{aligned} \tag{83}$$

$$\begin{aligned}
K &\equiv \int_1^\infty dz_1 dz_2 f(z_1) f(z_2) \frac{1}{z_1 + z_2} \frac{z_2^2}{z_2^2 - y^2} \\
&= \pi \left[\left(\frac{1}{8y^6} + \frac{19}{48y^4} + \frac{9}{80y^2} \right) + \sin^{-1}(y) \left(-\frac{1}{8y^7} - \frac{3}{8y^5} + \frac{1}{2y} \right) \right. \\
&\quad + \sin^{-1}(y) (1-y^2)^{1/2} \left(-\frac{1}{8y^7} - \frac{7}{16y^5} - \frac{3}{8y^3} \right) \\
&\quad \left. + (1-y^2)^{1/2} \left(\frac{1}{8y^6} + \frac{11}{24y^4} + \frac{5}{12y^2} \right) \right].
\end{aligned} \tag{84}$$

Using them, we have the following results for $y \leq 1$:

$$\begin{aligned}
&-2y \frac{d}{dy^2} H + (\ln(y)(2y^2 \frac{d}{dy^2} + 1) + 1)G \\
&= \frac{1}{2y^4} - \frac{2}{y^4} \ln(y) + \frac{5}{6y^2} - \frac{11}{6y^2} \ln(y) + \pi \left(\frac{\ln(2)}{y^5} + \frac{3\ln(2)}{4y^3} - \frac{1}{4y^5} - \frac{5}{8y^3} \right) \\
&\quad + g_2(1-y^2)^{1/2} \left(\frac{2}{y^5} + \frac{2}{y^3} \right) + g_2(1-y^2)^{-1/2} \left(\frac{1}{2y^3} + \frac{1}{y} \right) + g_1(1-y^2)^{1/2} \left(-\frac{1}{2y^5} - \frac{1}{y^3} \right),
\end{aligned} \tag{85}$$

$$\begin{aligned}
\frac{d}{dy} (J - yG) &= \frac{2}{y^4} + \frac{11}{6y^2} + \pi \left(-\frac{1}{y^5} - \frac{3}{4y^3} \right) + g_1(1-y^2)^{1/2} \left(-\frac{2}{y^5} - \frac{2}{y^3} \right) \\
&\quad + g_1(1-y^2)^{-1/2} \left(-\frac{1}{2y^3} - \frac{1}{y} \right),
\end{aligned} \tag{86}$$

$$\begin{aligned}
& (y \frac{d}{dy} + 1)(-y^2 G^2) - \frac{d}{dy}(K - y^2 G J) \\
&= \frac{7}{4y^6} + \frac{13}{3y^4} + \frac{85}{36y^2} + \pi(-\frac{2}{5y^3}) + \pi^2(-\frac{7}{16y^8} - \frac{15}{16y^6} + \frac{1}{4y^2}) \\
&+ (1 - y^2)^{-1/2} g_1(-\frac{7}{2y^7} - \frac{19}{3y^5} + \frac{13}{6y^3} + \frac{11}{3y}) + g_1^2(\frac{7}{4y^8} + \frac{15}{4y^6} - \frac{1}{y^2}), \tag{87}
\end{aligned}$$

where

$$g_1 = \sin^{-1}(y) - \frac{\pi}{2} = -\cos^{-1}(y), \tag{88}$$

and

$$\begin{aligned}
g_2 &= \ln(y) \sin^{-1}(y) - \frac{\pi}{2} \ln(1 + (1 - y^2)^{1/2}) \\
&= -\ln(y) \cos^{-1}(y) - \frac{\pi}{2} \ln(\frac{1}{y} + ((\frac{1}{y})^2 - 1)^{1/2}). \tag{89}
\end{aligned}$$

This completes our evaluation of the expectation values of various pieces of potentials into simple functions. Please note that g_1, g_2 and $(1 - y^2)^{1/2}$ appear together in the correct combinations to allow us to analytically continue the energy shifts into real functions on the proper branch for $y \geq 1$. They are given by the substitutions

$$\frac{\cos^{-1}(y)}{(1 - y^2)^{1/2}} \quad y \leq 1 \quad \rightarrow \quad \frac{\ln(y + (y^2 - 1)^{1/2})}{(y^2 - 1)^{1/2}} \quad y \geq 1, \tag{90}$$

and

$$\frac{\ln(\frac{1}{y} + ((\frac{1}{y})^2 - 1)^{1/2})}{((\frac{1}{y})^2 - 1)^{1/2}} \quad y \leq 1 \quad \rightarrow \quad \frac{\cos^{-1}(\frac{1}{y})}{(1 - (\frac{1}{y})^2)^{1/2}} \quad y \geq 1. \tag{91}$$

We have a complete analytical result for the single insertion of the potential to account for the finite charm mass effects for all values of y . Some of the integrals were not given in analytical forms by other authors and can be calculated numerically [6]. The values agree with ours within numerical accuracy, although we are somewhat unsure how the numerical integration programs decide on what branch to follow for $y \geq 1$.

B. Potential Terms and Energy Shifts for Double Insertions

In the next-next leading order, we have energy shifts due to double insertions of V_{charm}^{NLO} and $V_{massless}^{NLO}$ of Eqs.(59) and (61), respectively. For a state with wave function $\psi_{E_{n=1}}$ and perturbing potential \tilde{V} , the shift is given by

$$\Delta E_{double \text{ insertion}} = - \int d^3 \vec{x} \, d^3 \vec{y} \, \psi_{E_{n=1}}^\dagger(\vec{x}) \tilde{V}(x) \text{Lim}_{E \rightarrow E_{n=1}} G(\vec{x}, \vec{y}; E) \tilde{V}(y) \psi_{E_{n=1}}(\vec{y}). \tag{92}$$

Note that the regularization applies to the Green's function only. We shall discuss this point later on when we compare results. We write

$$\begin{aligned}
\tilde{V}(x) &= \frac{1}{2\pi^2} \int d^3\vec{k}_1 e^{i\vec{k}_1 \cdot \vec{x}} V(k_1^2), \\
&= \left(\frac{1}{2\pi^2}\right) \frac{2\pi}{ix} \int_0^\infty dk_1 k_1 (e^{ikx} - e^{-ikx}) V(k_1^2) \\
&= \left(\frac{1}{2\pi^2}\right) \frac{2\pi}{ix} \int_{-\infty}^\infty dk_1 k_1 e^{ikx} V(k_1^2)
\end{aligned} \tag{93}$$

and a similar expression for $\tilde{V}(y)$ with $k_1 \rightarrow k_2$. Likewise, we express

$$\psi(\vec{x})^\dagger = Y_{lm}^\dagger(\Omega_x) \left(\frac{1}{x}\right) \left(\frac{1}{2\pi}\right)^{1/2} \int_{-\infty}^\infty dp e^{ipx} \gamma_l^l(p), \tag{94}$$

and for $\psi(\vec{y})$ with $p \rightarrow p'$. Upon using the addition theorem

$$P_l\left(\frac{\vec{x} \cdot \vec{y}}{xy}\right) = \frac{4\pi}{2l+1} \sum_m Y_{lm}^\dagger(\Omega_x) Y_{lm}(\Omega_y), \tag{95}$$

to carry out the angular integration of \vec{x} and \vec{y} , we arrive at

$$\begin{aligned}
\Delta E_{double \text{ insertion}} &= -\frac{8\pi^2}{(2\pi^2 i)^2} \int_0^\infty dx \int_0^\infty dy \int_{-\infty}^\infty dk_1 k_1 \int_{-\infty}^\infty dk_2 k_2 \int_{-\infty}^\infty dp \int_{-\infty}^\infty dp' \\
&\times e^{ik_1 x} e^{ik_2 y} e^{ipx} e^{ip'y} \gamma_l^l(p) \gamma_l^l(p') V(k_1^2) V(k_2^2) G_l(x, y; E).
\end{aligned} \tag{96}$$

Now we specialize to the ground state given by Eqs.(54) and (55). We integrate over x and y, by using

$$\int_0^\infty dx e^{i(k_1+p+p_1)x} = i \frac{1}{k_1 + p + p_1}, \tag{97}$$

and Eq.(45), which give

$$\begin{aligned}
\Delta E_{double \text{ insertion}} &= \frac{2m_b}{(2\pi^2)^2} \frac{\kappa_1^3}{\kappa_0} \left(\frac{1}{2\pi i}\right)^2 \int_0^1 d\rho \rho^{-1-\nu} \\
&\times \int_{-\infty}^\infty dk_1 k_1 \int_{-\infty}^\infty dk_2 k_2 \int_{-\infty}^\infty dp \int_{-\infty}^\infty dp' \int_{-\infty}^\infty dp_1 \int_{-\infty}^\infty dp_2 \\
&\times \left(\frac{1}{p - i\kappa_1}\right)^2 \left(\frac{1}{p' - i\kappa_1}\right)^2 \frac{1}{k_1 + p + p_1} \frac{1}{k_2 + p' + p_2} \ln\left(\frac{bc}{ad}\right) V(k_1^2) V(k_2^2) \\
&= \frac{2m_b}{(2\pi^2)^2} \frac{\kappa_1^3}{\kappa_0} \int_0^1 d\rho \rho^{-1-\nu} \int_{-\infty}^\infty dk_1 k_1 \int_{-\infty}^\infty dk_2 k_2 \int_{-\infty}^\infty dp_1 \int_{-\infty}^\infty dp_2 \\
&\times \left(\frac{1}{k_1 + p_1 + i\kappa_1}\right)^2 \left(\frac{1}{k_2 + p_2 + i\kappa_1}\right)^2 \ln\left(\frac{bc}{ad}\right) V(k_1^2) V(k_2^2).
\end{aligned} \tag{98}$$

To organize our calculation better in what follows and so as not to have to track the branch cuts of products of logarithmic functions, we shall write

$$\begin{aligned}
V_{charm}^{NLO}(k^2) &= \left(-\frac{4}{3}\alpha_s\right) T_F \alpha_s \frac{2}{3\pi} \text{Lim}_{\mu_i \rightarrow 0} \left(\int_1^\infty dz \frac{f(z)}{k^2 + 4m^2 z^2} - \frac{1}{2} \int_0^1 \frac{dt}{t} \frac{1}{k^2 + \mu_i^2/t} \right. \\
&\quad \left. + \frac{1}{k^2} \left(\frac{1}{2} \ln\left(\frac{m^2}{\mu_i^2}\right) + \frac{5}{6} \right) \right),
\end{aligned} \tag{99}$$

and

$$V_{massless}^{NLO}(k^2) = (-\frac{4}{3}\alpha_s)\frac{\alpha_s}{4\pi}Lim_{\mu_i \rightarrow 0}(-\beta_0 \int_0^1 \frac{dt}{t} \frac{1}{k^2 + \mu_i^2/t} + \frac{1}{k^2}(-\beta_0 \ln(\frac{\mu_i^2}{\mu^2}) + a_1)). \quad (100)$$

Therefore, it is clear that after we calculate the energy shift due to

$$V_1(k^2) = (-\frac{4}{3}\alpha_s)(\alpha_s T_F \frac{2}{3\pi}) \int_1^\infty dz f(z) \frac{1}{k^2 + \bar{z}^2}, \quad \bar{z} = 2mz, \quad (101)$$

we can make minor changes on the spectral density and take $\bar{z}^2 \rightarrow \mu_i^2/t$ or $\bar{z} \rightarrow 0$ to get the other contributions. This is what we are going to do immediately.

The integration over k_1 in Eq.(98) gives

$$\int_{-\infty}^\infty dk_1 k_1 \frac{1}{k_1^2 + \bar{z}_1^2} \left(\frac{1}{k_1 + p_1 + i\kappa_1} \right)^2 = i\pi \left(\frac{1}{p_1 + i(\kappa_1 + \bar{z}_1)} \right)^2, \quad (102)$$

and a similar result for k_2 . This leads to integrations over p_1 and p_2 , which give a factor of

$$(2\pi i)^2 \frac{d^2}{dp_1 dp_2} \ln\left(\frac{bc}{ad}\right), \quad (103)$$

evaluated at $p_1 = -i(\kappa_1 + \bar{z}_1)$ and $p_2 = -i(\kappa_1 + \bar{z}_2)$.

We are interested in the limit of

$$p_0 = Lim_{\epsilon \rightarrow 0} i\kappa_1(1 + \epsilon), \quad \epsilon = 1 - \nu. \quad (104)$$

Thus in the calculation of the energy shift, we shall keep only the ϵ^0 and the $\frac{1}{\epsilon}$ terms. Since the ρ integration will produce the $\frac{1}{\epsilon}$ pole, we must keep terms to order ϵ^1 in the integrand as well. Now it is also clear that all terms of order $\epsilon\rho^n$ with $n \geq 2$ can be dropped. We shall show later on that the $\frac{1}{\epsilon}$ terms cancel, because we are interested in the subtracted propagator

$$Lim_{E \rightarrow E_{n=1}} (-G(\vec{x}, \vec{y}; E) - |E_{n=1} > \frac{1}{E - E_{n=1}} < E_{n=1}|), \quad (105)$$

to obtain the regulated level shift.

Carrying out the differentiation and evaluating at the value of $p_{1,2}$ as discussed, we find

$$\begin{aligned} \frac{d^2}{dp_1 dp_2} \ln\left(\frac{bc}{ad}\right) = & \rho \left[-\frac{4\kappa_1^2}{((2\kappa_1 + \bar{z}_1)(2\kappa_1 + \bar{z}_2) - \rho\bar{z}_1\bar{z}_2)^2} - \epsilon \frac{8\kappa_1^2}{(2\kappa_1 + \bar{z}_1)^2(2\kappa_1 + \bar{z}_2)^2} \right. \\ & \left. + \epsilon \frac{8\kappa_1^3(2\kappa_1 + \bar{z}_1 + 2\kappa_1 + \bar{z}_2)}{(2\kappa_1 + \bar{z}_1)^3(2\kappa_1 + \bar{z}_2)^3} \right]. \end{aligned} \quad (106)$$

We are now faced with an integral

$$I_\rho \equiv -4\kappa_1^2 \int_0^1 d\rho \rho^{-\nu} \left[\frac{1}{((2\kappa_1 + \bar{z}_1)(2\kappa_1 + \bar{z}_2) - \rho \bar{z}_1 \bar{z}_2)^2} + \epsilon \frac{2}{(2\kappa_1 + \bar{z}_1)^2 (2\kappa_1 + \bar{z}_2)^2} - \epsilon \frac{2\kappa_1(2\kappa_1 + \bar{z}_1 + 2\kappa_1 + \bar{z}_2)}{(2\kappa_1 + \bar{z}_1)^3 (2\kappa_1 + \bar{z}_2)^3} \right], \quad (107)$$

which can be easily calculated by adding and subtracting the terms in the square brackets at $\rho = 0$. Putting these pieces together, we obtain

$$\begin{aligned} \Delta E(V_1 V_1) &= 2m_b \frac{\kappa_1^3}{\kappa_0} \left(\left(\frac{4}{3} \alpha_s \right) (\alpha_s T_F \frac{2}{3\pi}) \right)^2 \\ &\times \int_1^\infty dz_1 f(z_1) \int_1^\infty dz_2 f(z_2) 4\kappa_1^2 \left\{ \frac{1}{(2\kappa_1 + \bar{z}_1)^2 (2\kappa_1 + \bar{z}_2)^2} \right. \\ &\times \left[-\frac{1}{\epsilon} + \text{Ln} \left(\frac{(2\kappa_1 + \bar{z}_1)(2\kappa_1 + \bar{z}_2) - \bar{z}_1 \bar{z}_2}{(2\kappa_1 + \bar{z}_1)(2\kappa_1 + \bar{z}_2)} \right) \right. \\ &\left. \left. - \frac{\bar{z}_1 \bar{z}_2}{(2\kappa_1 + \bar{z}_1)(2\kappa_1 + \bar{z}_2) - \bar{z}_1 \bar{z}_2} \right] - \frac{2}{(2\kappa_1 + \bar{z}_1)^2 (2\kappa_1 + \bar{z}_2)^2} \right. \\ &\left. + 2\kappa_1 \left(\frac{1}{(2\kappa_1 + \bar{z}_1)^2 (2\kappa_1 + \bar{z}_2)^3} + \frac{1}{(2\kappa_1 + \bar{z}_1)^3 (2\kappa_1 + \bar{z}_2)^2} \right) \right\}. \quad (108) \end{aligned}$$

There remain two items to be settled. We first expand

$$\kappa_0^{-1} = \kappa_1^{-1} (1 - \epsilon) \quad (109)$$

in Eq.(108) and then perform a subtraction as indicated in Eq.(105) because the ground state should not be included in the propagator. This yields the subtraction term

$$\begin{aligned} & - \int d^3 \vec{x} \int d^3 \vec{y} \psi^\dagger(\vec{x})_{E_{n=1}} \tilde{V}_1(x) \psi(\vec{x})_{E_{n=1}} \frac{1}{E - E_{n=1}} \psi^\dagger(\vec{y})_{E_{n=1}} \tilde{V}_1(y) \psi(\vec{y})_{E_{n=1}} \\ &= \frac{m_b}{2\kappa_1^2} \left(\frac{1}{\epsilon} \right) \left(1 - \frac{3}{2} \epsilon \right) (\Delta E^{NLO})^2, \quad (110) \end{aligned}$$

where

$$(\Delta E)^{NLO} = \left(-\frac{4}{3} \alpha_s \right) (T_F \alpha_s \frac{2}{3\pi}) (4\kappa_1^3) \int_1^\infty dz f(z) \frac{1}{(2\kappa_1 + \bar{z})^2}. \quad (111)$$

The end result is

$$\begin{aligned} \Delta E(V_1 V_1)^{reg} &= 2m_b \kappa_1^2 \left(\left(\frac{4}{3} \alpha_s \right) (\alpha_s T_F \frac{2}{3\pi}) \right)^2 \\ &\times \int_1^\infty dz_1 f(z_1) \int_1^\infty dz_2 f(z_2) 4\kappa_1^2 \left\{ \frac{1}{(2\kappa_1 + \bar{z}_1)^2 (2\kappa_1 + \bar{z}_2)^2} \right. \\ &\times \left[-\frac{1}{2} + \text{Ln} \left(\frac{(2\kappa_1 + \bar{z}_1)(2\kappa_1 + \bar{z}_2) - \bar{z}_1 \bar{z}_2}{(2\kappa_1 + \bar{z}_1)(2\kappa_1 + \bar{z}_2)} \right) \right. \end{aligned}$$

$$\left. -\frac{\bar{z}_1\bar{z}_2}{(2\kappa_1+\bar{z}_1)(2\kappa_1+\bar{z}_2)-\bar{z}_1\bar{z}_2} \right] - \frac{2}{(2\kappa_1+\bar{z}_1)^2(2\kappa_1+\bar{z}_2)^2} + 2\kappa_1 \left(\frac{1}{(2\kappa_1+\bar{z}_1)^2(2\kappa_1+\bar{z}_2)^3} + \frac{1}{(2\kappa_1+\bar{z}_1)^3(2\kappa_1+\bar{z}_2)^2} \right) \Big\}, \quad (112)$$

As a check that our regularization is correct, we look into the modified Coulomb potential

$$\tilde{V}(\vec{x}) = -\frac{4}{3}\alpha_s(1+\delta)\frac{1}{x}, \quad (113)$$

with the term proportional to δ treated as a perturbation, which produces the ground energy

$$E_{ground} = -\frac{m_b}{4}\left(\frac{4}{3}\alpha_s\right)^2(1+\delta)^2. \quad (114)$$

The δ^2 term is recovered from Eq.(112) by setting $\bar{z}_{1,2} \rightarrow 0$ and requiring the spectral density to satisfy $(\alpha_s T_F \frac{2}{3\pi}) \int dz f(z) \rightarrow 1$.

We shall take this as our standard subtraction, which will be applied to Eq.(108) and remaining energy shifts, by the operation

$$\kappa_0 \rightarrow \kappa_1, \quad \frac{1}{\epsilon} \rightarrow \frac{1}{2}. \quad (115)$$

To finish the calculation due to Eq.(99), we define

$$V_{charm}^{NLO}(k^2) = V_1(k^2) + V_2(k^2) + V_3(k^2), \quad (116)$$

$$V_2(k^2) = \left(-\frac{4}{3}\alpha_s\right)T_F\alpha_s\frac{2}{3\pi}Lim_{\mu_i \rightarrow 0}\left(-\frac{1}{2}\int_0^1 \frac{dt}{t} \frac{1}{k^2 + \mu_i^2/t}\right), \quad (117)$$

$$V_3(k^2) = \left(-\frac{4}{3}\alpha_s\right)T_F\alpha_s\frac{2}{3\pi}Lim_{\mu_i \rightarrow 0}\frac{1}{k^2}\left(\frac{1}{2}ln\left(\frac{m^2}{\mu_i^2}\right) + \frac{5}{6}\right), \quad (118)$$

and

$$bb = 2m_b\frac{\kappa_1^3}{\kappa_0}\left(\frac{4}{3}\alpha_s\left(\alpha_s T_F \frac{2}{3\pi}\right)\right)^2, \quad (119)$$

then the shift due to V_1V_2 is

$$\begin{aligned} \Delta E(2V_1V_2) = & 2(-1/2)bb \int_1^\infty dz_1 f(z_1) \int_0^1 \frac{dt}{t} 4\kappa_1^2 \left\{ \frac{1}{(2\kappa_1+\bar{z}_1)^2(2\kappa_1+\mu_i/\sqrt{t})^2} \right. \\ & \times \left[-\frac{1}{\epsilon} + Ln\left(\frac{(2\kappa_1+\bar{z}_1)(2\kappa_1+\mu_i/\sqrt{t})-\bar{z}_1\mu_i/\sqrt{t}}{(2\kappa_1+\bar{z}_1)(2\kappa_1+\mu_i/\sqrt{t})}\right) \right. \\ & \left. \left. - \frac{\bar{z}_1\mu_i/\sqrt{t}}{(2\kappa_1+\bar{z}_1)(2\kappa_1+\mu_i/\sqrt{t})-\bar{z}_1\mu_i/\sqrt{t}} \right] - \frac{2}{(2\kappa_1+\bar{z}_1)^2(2\kappa_1+\mu_i/\sqrt{t})^2} \right. \\ & \left. + 2\kappa_1 \left(\frac{1}{(2\kappa_1+\bar{z}_1)^3(2\kappa_1+\mu_i/\sqrt{t})^2} + \frac{1}{(2\kappa_1+\bar{z}_1)^2(2\kappa_1+\mu_i/\sqrt{t})^3} \right) \right\}. \quad (120) \end{aligned}$$

We perform the t integration to obtain

$$\Delta E(2V_1V_2) = bb \int_1^\infty dz f(z) \left\{ \frac{1}{(2\kappa_1 + \bar{z})^2} \left[2Li\left(\frac{\bar{z}}{2\kappa_1 + \bar{z}}\right) - 2\left(\frac{1}{2} + \ln\left(\frac{\mu_i}{2\kappa_1}\right)\right) - \frac{2}{\epsilon}(1 + \ln\left(\frac{\mu_i}{2\kappa_1}\right)) \right] + \frac{4\kappa_1}{(2\kappa_1 + \bar{z})^3}(1 + \ln\left(\frac{\mu_i}{2\kappa_1}\right)) \right\}. \quad (121)$$

Similarly, the V_1V_3 shift is arrived at by taking the zero mass limit of \bar{z}_2 , which leads to

$$\Delta E(2V_1V_3) = bb \int_1^\infty dz f(z) \left[\frac{1}{(2\kappa_1 + \bar{z})^2} \left(-\frac{2}{\epsilon} - 2 \right) + \frac{4\kappa_1}{(2\kappa_1 + \bar{z})^3} \right] \left(\frac{1}{2} \ln\left(\frac{m^2}{\mu_i^2}\right) + \frac{5}{6} \right). \quad (122)$$

It is important to note that $\ln(\mu_i)$'s cancel in Eqs.(121-122), as they must, because μ_i is introduced to facilitate our calculation. Physical results should not depend on it. Shifts due to other pieces are deduced in a similar way upon being careful not to interchange the $\mu_i \rightarrow 0$ limit and the t -integration. We have

$$\Delta E(V_2V_2 + 2V_2V_3 + V_3V_3) = bb \frac{1}{4\kappa_1^2} \left[-\frac{1}{\epsilon} \left(\frac{11}{6} + \ln\left(\frac{m}{2\kappa_1}\right) \right)^2 + \ln\left(\frac{m}{2\kappa_1}\right) + \frac{11}{6} - \left(\zeta_3 - \frac{\pi^2}{6} + 1 \right) \right], \quad (123)$$

and

$$\Delta E(2V_1(V_2 + V_3)) = bb \int_1^\infty dz f(z) \left[\frac{1}{(2\kappa_1 + \bar{z})^2} \left(2Li\left(\frac{\bar{z}}{2\kappa_1 + \bar{z}}\right) - \frac{2}{\epsilon} \left(\frac{11}{6} + \ln\left(\frac{m}{2\kappa_1}\right) \right) - 2\ln\left(\frac{m}{2\kappa_1}\right) - \frac{8}{3} \right) + \frac{4\kappa_1}{(2\kappa_1 + \bar{z})^3} \left(\ln\left(\frac{m}{2\kappa_1}\right) + \frac{11}{6} \right) \right]. \quad (124)$$

In a similar manner, we introduce

$$V_{massless}^{NLO}(k^2) = V_1'(k^2) + V_2'(k^2), \quad (125)$$

where

$$V_1'(k^2) = \left(-\frac{4}{3}\alpha_s \right) \frac{\alpha_s}{4\pi} Lim_{\mu_i \rightarrow 0} \left(-\beta_0 \int_0^1 \frac{dt}{t} \frac{1}{k^2 + \mu_i^2/t} \right), \quad (126)$$

and

$$V_2'(k^2) = \left(-\frac{4}{3}\alpha_s \right) \frac{\alpha_s}{4\pi} Lim_{\mu_i \rightarrow 0} \left(\frac{1}{k^2} \left(-\beta_0 \ln\left(\frac{\mu_i^2}{\mu^2}\right) + a_1 \right) \right), \quad (127)$$

and also

$$ab = 2m_b \frac{\kappa_1^3}{\kappa_0} \left(\frac{4}{3}\alpha_s \right)^2 (T_F \alpha_s \frac{2}{3\pi}) \left(\frac{\alpha_s}{4\pi} \right). \quad (128)$$

We have

$$\begin{aligned} \Delta E(2V_1(V'_1 + V'_2)) = & 2(ab) \int_1^\infty dz f(z) \left[\frac{1}{(2\kappa_1 + \bar{z})^2} \left(2\beta_0 Li\left(\frac{\bar{z}}{2\kappa_1 + \bar{z}}\right) \right. \right. \\ & - \frac{1}{\epsilon} \left(2\beta_0 + a_1 + 2\beta_0 \ln\left(\frac{\mu}{2\kappa_1}\right) \right) - 2\beta_0 \ln\left(\frac{\mu}{2\kappa_1}\right) - \beta_0 - a_1 \Big) \\ & \left. \left. + \frac{2\kappa_1}{(2\kappa_1 + \bar{z})^3} \left(2\beta_0 \ln\left(\frac{\mu}{2\kappa_1}\right) + 2\beta_0 + a_1 \right) \right] , \end{aligned} \quad (129)$$

and

$$\begin{aligned} \Delta E(2(V_2 + V_3)(V'_1 + V'_2)) = & 2(ab) \frac{1}{4\kappa_1^2} \left[-\frac{1}{\epsilon} \left(\frac{11}{6} + \ln\left(\frac{m}{2\kappa_1}\right) \right) \left(2\beta_0 + a_1 + 2\beta_0 \ln\left(\frac{\mu}{2\kappa_1}\right) \right) \right. \\ & \left. + \beta_0 \ln\left(\frac{m\mu}{(2\kappa_1)^2}\right) + \frac{17}{6}\beta_0 + \frac{a_1}{2} - 2\beta_0 \left(\zeta_3 - \frac{\pi^2}{6} + 1 \right) \right] . \end{aligned} \quad (130)$$

We see again that $\ln(\mu_i)$'s cancel. The subtracted results of Eqs.(121-130) as said are given by the prescription of Eq.(115). This finishes our double insertions. We have not been able to evaluate all the two dimensional integrals into simple functions as we could in section 4A. In fact, for $y=1$, some of these integrals produce the Catalan number, an indication that they are probably related to hyper-geometric functions. Our end result here agrees with that in ref.[6].

V. NUMERICAL RESULTS

In this section, we present some numerical results. The mass in Eq.(1) is the b quark pole mass M_b^{pole} and the charm quark mass used throughout is $\overline{\text{MS}}$ mass $m_c(\bar{m}_c)$. For our numerical work, we take

$$\bar{m}_c = 1.25 \text{ GeV}, \quad M_b^{pole} = 5.0 \text{ GeV}. \quad (131)$$

The typical energy scale involved is taken as $\mu = \frac{4}{3}\alpha_s M_b^{pole} = 2.0 \text{ GeV}$, at which the running coupling constant is evaluated to be

$$\alpha_s(2.0) = 0.30. \quad (132)$$

These give $y = 0.80$. The energy of 1S state of bottomonium due to the non-zero charm quark mass is shifted by

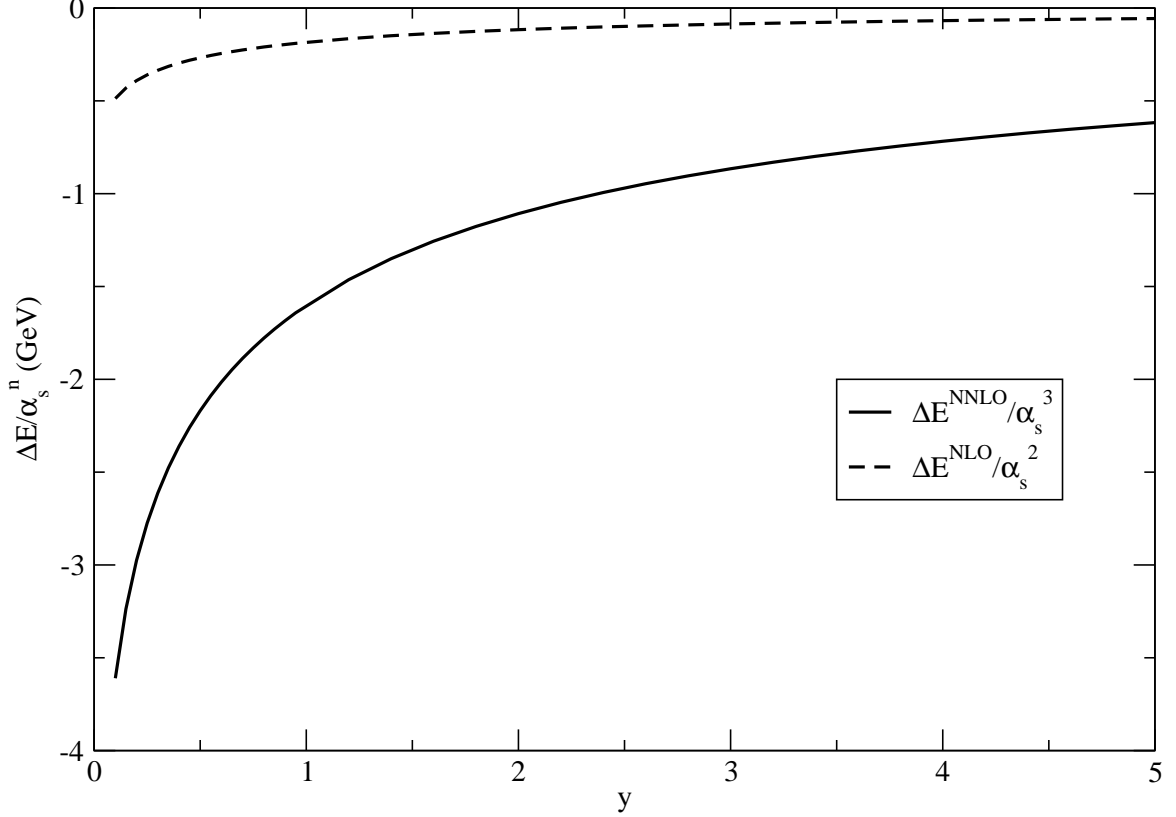


FIG. 3: This figure compares the behaviors of $\Delta E^{NNLO}/\alpha_s^3$ against $\Delta E^{NLO}/\alpha_s^2$ as functions of $y = \kappa_1/m_c$. The solid line represents $\Delta E^{NNLO}/\alpha_s^3$, while the dashed line represents $\Delta E^{NLO}/\alpha_s^2$.

$$\Delta E_{1S}^{NLO} = -18.9 \text{ MeV}, \quad \Delta E_{1S}^{NNLO} = -48 \text{ MeV}, \quad (133)$$

due to next leading order and next to next leading order corrections, respectively. Altogether, these amount to a shift of bottom quark 1S mass [17].

$$\Delta M_b^{1S} = -33 \text{ MeV}. \quad (134)$$

With our explicit expressions for energy shift, we can calculate it for all values of y , including $y > 1$. We display in Fig. 3 the behavior of $\Delta E^{NNLO}/\alpha_s^3$ and $\Delta E^{NLO}/\alpha_s^2$ as functions of y to succinctly summarize the intricate interplay of masses, by eliminating their

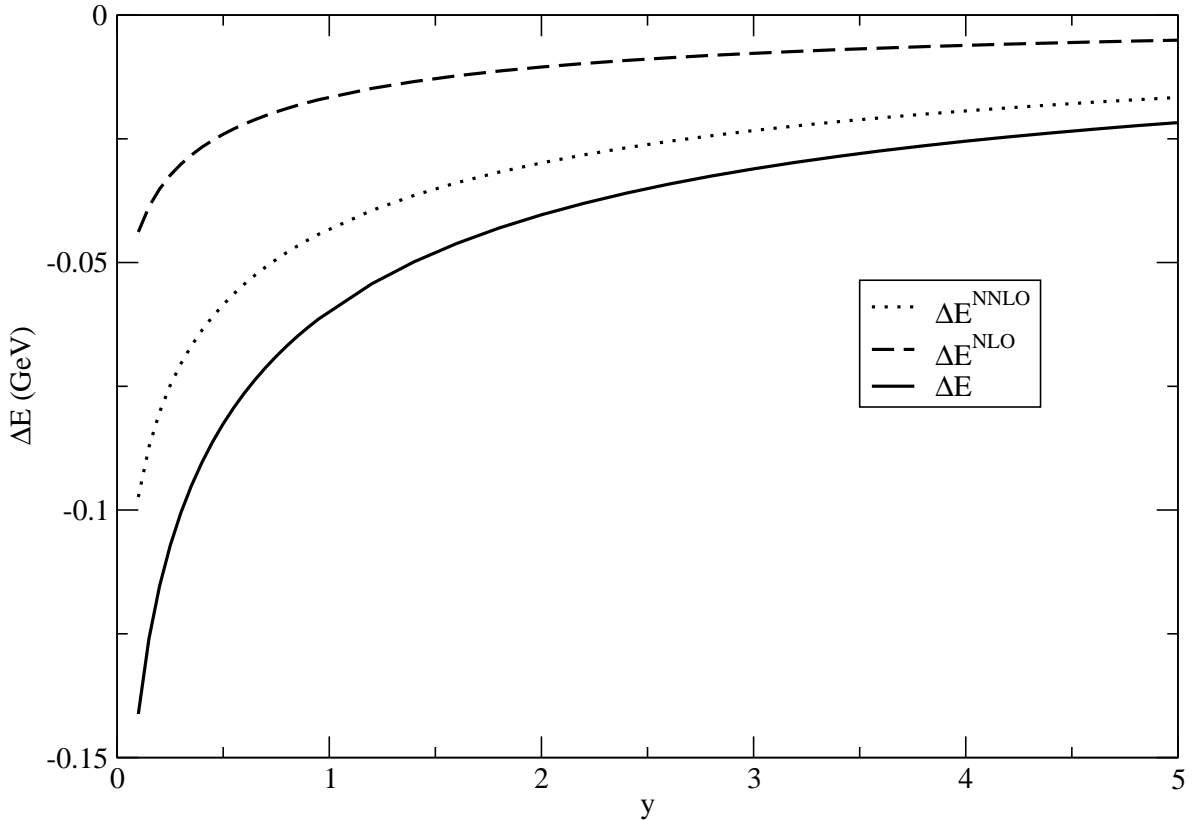


FIG. 4: The 1S level shifts due to the charm mass effects are shown as functions of y at NLO (dashed line) and NNLO (dotted line). The total contribution of NLO and NNLO is represented by the solid line.

dependence on the running coupling constant. In Fig. 4, we plot the NLO, NNLO and the total contribution to 1S level energy shift as functions of y .

Note that when $m_c \rightarrow 0$, which corresponds to $y \rightarrow \infty$, the energy shift due to double insertions tend to zero. This point was emphasized by Hoang [6], because the leading order effects of the charm potential (Eq.(59)) has no spatial dependence and the orthogonality of the wave functions which make up the propagator dictates this behavior.

The $t\bar{t}$ “energy level shift” due to non-vanishing bottom quark mass can also be easily

estimated. We use

$$M_t = 174 \text{ GeV}, \quad m_b = 4.2 \text{ GeV}, \quad \alpha_s(M_t) = 0.108, \quad (135)$$

which yield $y = 2.98$. Up to NNLO, the “1S energy level shift” due to the bottom quark mass effect reads

$$\Delta E = -25 \text{ MeV}, \quad (136)$$

which is suppressed by the smallness of the coupling constant as compared with bottomonium.

VI. CONCLUDING REMARKS

One motivation for this work is to give a formulation to treat bound state and threshold physics completely in momentum space. For performing detailed high order calculations, it seems that the momentum space may have a natural setting, because Feynman rules are normally derived and given there.

We have accomplished the construction of Coulomb wave functions for all quantum numbers. Our propagators are quite compact, which among other things replace sums over principal quantum numbers by a parametric integral. The limit as the energy of the propagator(s) approaches any of the bound state can be isolated easily.

We have applied this formalism to investigate the charm effects on the 1S bottomonium level shifts to the next-next leading order. Here, we have expressed all the single insertion results analytically in elementary functions. For double insertions, where the ground state is to be omitted as an intermediate state, it corresponds to a pole subtraction in $\frac{1}{\epsilon}$.

Clearly, our formalism is useful for other problems. We have, for example, cursorily looked into the shifts due to charm effects in the next leading order on arbitrary bottomonium energy levels. We find the needed technique to be a slight extension of what we shall present in the appendix. Since the results for the shifts are known [8], we shall not pursue it further. The S-states due to a linear potential can also be easily treated in this formulation.

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APPENDIX A: MATRIX ELEMENTS IN QUANTUM MECHANICS

We want to show how some matrix elements in quantum mechanics can be reproduced in our approach. Let us look at an integral for a fixed n

$$\begin{aligned} \int d\xi \frac{\tilde{\gamma}_l(\xi)}{\xi^s} \frac{\tilde{\gamma}_l(\xi)}{\xi^t} &= \int_{-\infty}^{\infty} dp \gamma_l^s(-p) \gamma_l^t(p) \\ &= \frac{A_l^2}{(i)^{s+t}} (-1)^{s+t} \frac{1}{(s-1)!} \frac{1}{(t-1)!} \int_{-\infty}^0 dp_1 p_1^{t-1} \int_{-\infty}^0 dp_2 p_2^{s-1} \\ &\quad \times \int_{-\infty}^{\infty} dp \frac{(p_1 + p + p_0)^{n-l-1} (p_2 - p + p_0)^{n-l-1}}{(p_1 + p - p_0)^{n+l+1} (p_2 - p - p_0)^{n+l+1}}. \end{aligned} \quad (A1)$$

Using the residue theorem, we have

$$\begin{aligned} \int d\xi \frac{\tilde{\gamma}_l(\xi)}{\xi^s} \frac{\tilde{\gamma}_l(\xi)}{\xi^t} &= \frac{A_l^2}{(i)^{s+t}} (-1)^{s+t} \frac{1}{(s-1)!} \frac{1}{(t-1)!} \int_{-\infty}^0 dp_1 p_1^{t-1} \int_{-\infty}^0 dp_2 p_2^{s-1} \\ &\quad \times \frac{2\pi i}{(n+l)!} \left(\frac{d}{dx} \right)^{n+l} \frac{(2p_0 + x)^{n-l-1} (p_1 + p_2 - x)^{n-l-1}}{(p_1 + p_2 - 2p_0 - x)^{n+l+1}} \Big|_{x=0}. \end{aligned} \quad (A2)$$

If $2(l+1) \geq s+t$, we can interchange the differentiation and the integrations over $p_{1,2}$. Then, Eq.(37) gives

$$\begin{aligned} \int d\xi \frac{\tilde{\gamma}_l(\xi)}{\xi^s} \frac{\tilde{\gamma}_l(\xi)}{\xi^t} &= \frac{A_l^2}{(i)^{s+t}} \frac{2\pi i}{(n+l)!} \frac{1}{\Gamma(s+t)} \left(\frac{d}{dx} \right)^{n+l} b^{n-l-1} \\ &\quad \times \int_0^{\infty} dp' \frac{p'^{s+t-1} (p' + x)^{n-l-1}}{(p' + b)^{n+l+1}} \Big|_{x=0} \\ &= (-1)^{s+t} \frac{A_l^2}{(i)^{s+t}} \frac{2\pi i}{(n+l)!} \sum_{i=0}^{n-l-1} \frac{(-2p_0)^{n-l-1-i} (n-l-1)!}{i! (n-l-1-i)!} \\ &\quad \times \sum_{j=0}^{s+t-1} \frac{(-1)^{1+j}}{j! (s+t-1-j)!} \frac{1}{n+l-i-j} \left(\frac{d}{dx} \right)^{n+l} b^{s+t-2l+i-2} \Big|_{x=0}, \end{aligned} \quad (A3)$$

where $b = 2p_0 + x$. Note that in most cases, only a small number of terms will survive the differentiation. For example, we can check the normalization A_l by setting $s = t = l$, which leads to

$$\sum_{j=0}^{2l-1} \frac{(-1)^{1+j}}{j!(2l-1-j)!} \frac{1}{n+l-i-j} = \frac{1}{(n-i+l)(n-i+l-1)\dots(n-i-l+1)}, \quad (\text{A4})$$

and then

$$\begin{aligned} \int_0^\infty d\xi u(\xi)^2 &= \int_0^\infty d\xi \frac{\tilde{\gamma}_l(\xi)}{\xi^l} \frac{\tilde{\gamma}_l(\xi)}{\xi^l} = \int_{-\infty}^\infty dp \gamma_l^l(p) \gamma_l^l(-p) \\ &= \frac{A_l^2}{(i)^{2l}} \frac{2\pi i}{(n+l)!} \sum_{i=0}^{n-l-1} (-2p_0)^{n-l-1-i} \frac{(n-l-1)!(n-i-l)}{(n-i+l)!i!} \\ &\quad \times \left(\frac{d}{dx}\right)^{n+l} b^{i-2} \Big|_{x=0}. \end{aligned} \quad (\text{A5})$$

Clearly only $i = 0$ and $i = 1$ contribute to the sum because of the d/dx operation. We have after some simple algebra

$$\begin{aligned} \int_0^\infty d\xi u(\xi)^2 &= \int_0^\infty d\xi \frac{\tilde{\gamma}_l(\xi)}{\xi^l} \frac{\tilde{\gamma}_l(\xi)}{\xi^l} \\ &= \frac{A_l^2}{(i)^{2l}} \left(\frac{1}{2\kappa}\right)^{2l+3} \frac{2\pi}{(n+l)!} (n-l-1)!(2n) \\ &= 1, \end{aligned} \quad (\text{A6})$$

as it must.

Next we consider $s + t = 2l + 1$, which will give us the expectation value of $1/\xi$. This time we use in Eq.(A3)

$$\sum_{j=0}^{2l} \frac{(-1)^{1+j}}{j!(2l-j)!} \frac{1}{n+l-i-j} = \frac{-1}{(n-i+l)(n-i+l-1)\dots(n-i-l)}, \quad (\text{A7})$$

which gives

$$\begin{aligned} \int_0^\infty d\xi u(\xi) \frac{1}{\xi} u(\xi) &= \int_0^\infty d\xi \frac{\tilde{\gamma}_l(\xi)}{\xi^l} \frac{1}{\xi} \frac{\tilde{\gamma}_l(\xi)}{\xi^l} = \int_{-\infty}^\infty dp \gamma_l^{l+1}(p) \gamma_l^l(-p) \\ &= \frac{A_l^2}{(i)^{2l+1}} \frac{2\pi i}{(n+l)!} \sum_{i=0}^{n-l-1} (-2p_0)^{n-l-1-i} \frac{(n-l-1)!}{(n-i+l)!i!} \\ &\quad \times \left(\frac{d}{dx}\right)^{n+l} b^{i-1} \Big|_{x=0}. \end{aligned} \quad (\text{A8})$$

There is only one term $i=0$ in the sum which is not annihilated by d/dx and we come up with

$$\begin{aligned}\int_0^\infty d\xi \, u(\xi) \frac{1}{\xi} u(\xi) &= A_l^2 2\pi \frac{(n-l-1)!}{(n+l)!} \left(\frac{1}{2\kappa}\right)^{2l+2} \\ &= \frac{1}{n^2 a},\end{aligned}\tag{A9}$$

which agrees with a well-known result.

As we stated earlier, to interchange the integration and the differentiation operations in Eq.(A3), it is necessary that the condition $2(l+1) \geq s+t$ should be satisfied. For the case $s+t = 2l+2$, which is relevant for the expectation value of $1/\xi^2$, we must treat it differently. Thus, we write

$$\int_0^\infty d\xi \, \frac{\tilde{\gamma}_l(\xi)}{\xi^{l+1}} \frac{\tilde{\gamma}_l(\xi)}{\xi^{l+1}} = \frac{A_l^2}{(i)^{2l+2}} \frac{2\pi i}{(n+l)!} \frac{1}{(2l+1)!} B,\tag{A10}$$

where

$$B = \int_0^\infty dp' \, p'^{2l+1} \left(\frac{d}{dx}\right)^{n+l} b^{n-l-1} \frac{(p'+x)^{n-l-1}}{(p'+b)^{n+l+1}} \Big|_{x=0}.\tag{A11}$$

We rewrite

$$p' + x = p' + b - 2p_0,\tag{A12}$$

and expand in binomial the numerator

$$\begin{aligned}\frac{(p'+x)^{n-l-1}}{(p'+b)^{n+l+1}} &= \frac{1}{(p'+b)^{2l+2}} + \frac{(n-l-1)(-2p_0)}{(p'+b)^{2l+3}} \\ &+ \frac{(n-l-1)(n-l-2)(-2p_0)^2}{2(p'+b)^{2l+4}} + \dots\end{aligned}\tag{A13}$$

Only the first term will be non-vanishing after the d/dx differentiations, since all the others terms are convergent enough that we can interchange the integration and differentiation operations and are proportional to $(d/dx)^{n+l} b^k$, $k < n+l$. Then effectively

$$B = \int_0^\infty dp' \, p'^{2l+1} \left(\frac{d}{dx}\right)^{n+l} \frac{b^{n-l-1}}{(p'+b)^{2l+2}}.\tag{A14}$$

After examining a few values of n and l , one can easily convince oneself that

$$B = -(n-l-1)!(2l)! b^{-(2l+1)},\tag{A15}$$

and thus

$$\int_0^\infty d\xi \frac{\tilde{n}(\xi)}{\xi^{l+1}} \frac{\tilde{n}(\xi)}{\xi^{l+1}} = \frac{1}{n^3 a^2} \frac{1}{l + 1/2}, \quad (\text{A16})$$

which again is a well-known result.

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 - [17] There is a strong dependence on the scale μ . Our choice is $\mu = 2.0 \text{ GeV}$. As a contrast, for $\bar{m}_c = 1.5 \text{ GeV}$, $M_b^{\text{pole}} = 5 \text{ GeV}$, and $\alpha_s = 0.216$ at $\mu = 4.7 \text{ GeV}$, one would get $\Delta M_b^{1S} = -16 \text{ MeV}$, close to what was obtained in [6]. Roughly speaking, our lower choice of μ enhances NLO by 9/4 and NNLO by 27/8 due to α_s . The dependence on μ for \overline{MS} b mass is much

weaker. See [7] for a discussion.